AD-A151 763 THEORY OF ELECTRON-IMPACT ATOMIC IONIZATION CROSS SECTIONS(U) OREGON UNIV EUGENE M D GIRARDEAU MAR 85 N00014-81-K-0759 1/1

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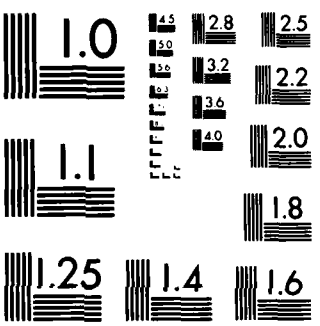

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7. AUTHOR(s): Marvin D. Girardeau	8. CONTRACT OR GRANT NUMBER(s): N00014-81-K-0759
9. PERFORMING ORGANIZATION NAME AND ADDRESS: Department of Physics and Institutes of Chemical Physics and Theoretical Science, University of Oregon, Eugene, OR 97403	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS: Program Element: 61153N Project-Task Area: RR011-03-02 Work Unit: NR 394-055
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19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Atomic collisions, charge exchange cross sections, electron impact ionization cross sections

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Work performed during the period 1 July 1984 - 30 June 1985 on Contract N00014-81-K-0759 is summarized.

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ANNUAL SUMMARY REPORT

for

1 July 1984 through 30 June 1985

for

Contract N00014-81-K-0759

Task No. NR 394-055

Title of Contract:

Theory of Electron-Impact Atomic Ionization Cross Sections

Name of Principal Investigator:

Marvin D. Girardeau

Name of Organization:

Department of Physics and
Institutes of Chemical Physics and Theoretical Science,
University of Oregon

Address of Organization:

Eugene, Oregon 97403

A. Description of Problem

The research underway is concerned with both the general theory and detailed numerical calculations of differential cross sections for charge exchange and electron impact ionization ocurring in collisions of simple atomic, ionic, and molecular species. Our general approach is based on systematic application of the "Fock-Tani representation" developed by the Principal Investigator and his co-workers. References to our publications in this area are contained in the proposal for renewal of this contract. Calculations carried out during the current contract period 1 July 1984-30 June 1985 are for the charge-exchange reactions $D^+ + H \rightarrow D + H^+$, $D^+ + H \rightarrow (HD^+)^* \rightarrow D + H^+$ [where $(HD^+)^*$ is a predissociating molecular ion giving resonance contributions], and $H^+ + H \rightarrow H + H^+$, as well as for the electron-impact ionization process $e + H \rightarrow H^+ + e + e$. The Fock-Tani representation used leads to a modified Born expansion which includes more physics (specifically, certain orthogonalization corrections) in first order than the conventional first Born approximation, and hence extends the validity of the first-order theory to lower energies. In order to further extend the validity into regions where initial/final state interactions are important, we are evaluating monopole-induced dipole contributions to the second Born approximation.

B. Progress since 1 July 1984

Numerical calculations of differential cross sections for

the charge-exchange reaction $D^+ + H \rightarrow D + H^+$ through first order in our "Fock-Tani Born expansion" have already been carried out and will be included in a manuscript currently being written, along with the results of similar numerical calculations for $H^+ + H \rightarrow H + H^+$ which will be completed by 15 March 1985. Contributions of initial/final state interactions to these cross sections are currently being investigated by J. Straton, a Research Assistant (graduate student) on this project, who expects to complete his Ph.D. dissertation during late summer or fall 1985. Preliminary analytical work on reduction of dimensionality of integrals occurring in the "Fock-Tani first Born approximation" for $e + H \rightarrow H^+ + e + e$ has been carried out as a preliminary to the numerical evaluation. Analytical work cn resonance contributions to reactions of the form $D^+ + H(nlm) \rightarrow (HD^+)^* \rightarrow D(n'l'm') + H^+$ is underway.

C. Manuscripts published and submitted.

For publications and manuscripts submitted up to 30 September 1984 please see the Publications/Patents/Presentations/Honors Report attached as an appendix of this report. In addition, the following manuscripts have been submitted since 30 September 1984:

1. M.D. Girardeau, "Lippmann-Schwinger theory of half-collision cross sections", Phys. Rev. Lett.
2. M.D. Girardeau, "Distorted wave amplitudes, DWBA, and self energies in the Fock-Tani theory of rearrangement collisions", Phys. Rev. A.

Appendix

OFFICE OF NAVAL RESEARCH

PUBLICATIONS / PATENTS / PRESENTATIONS / HONORS REPORT

for

1 October 1983 through 30 September 1984

for

Contract N00014-81-K-0759

Task No. NR 394-055

Title of Contract:

Theory of Electron-Impact Atomic Ionization Cross Sections

Name of Principal Investigator:

Marvin D. Girardeau

Name of Organization:

Department of Physics and
Institutes of Chemical Physics and Theoretical Science,
University of Oregon

Address of Organization:

Eugene, Oregon 97403

PAPERS SUBMITTED TO REFEREED JOURNALS
(Not Yet Published)

M.D. Girardeau and H. Barentzen, "Boson representation for a system of fermions in terms of an overcomplete geminal basis," J. Math. Phys.

H. Kupka, M.D. Girardeau, C.I. Ivanov and H. Barentzen, "Fock-Tani representation for molecular predissociation," J. Chem. Phys.

Note: The work represented by the above papers was performed during the visit of M.D. Girardeau in the Max Planck Institut fur Strahlenchemie, Mulheim a.d. Ruhr, West Germany, during summer 1984 as a Senior U.S. Scientist Awardee of the Alexander von Humboldt-Stiftung. All expenses (including Professor Girardeau's salary) were borne by the Humboldt Foundation and Max Planck Institut, and publication charges will be paid by them. The papers are, nevertheless, listed here since they are in the general area of research of this ONR contract and are expected to contribute indirectly to the ongoing research program at the University of Oregon.

PAPERS PUBLISHED IN REFEREED JOURNALS

C.F. Hart and M.D. Girardeau, "New variational principle for decaying states," Phys. Rev. Lett. 51, 1725 (1983).

M.D. Girardeau, "Reduction of a quantum n-body problem to an (n-1)-body problem," Phys. Rev. A 28, 3635 (1983).

(Note: The two above publications and the research leading to them were funded by this ONR contract. There was no other support except for the P.I.'s academic year salary from the University of Oregon.)

H. Barentzen and M.D. Girardeau, "Completeness of pair wave functions," Phys. Lett. 102A, 393 (1984).

(Note: This work was funded entirely by the Max Planck Institut fur Strahlenchemie, which paid all expenses of Dr. Barentzen's visit to the University of Oregon for a five-month period commencing March 1983, including his salary while here.)

BOOKS (AND SECTIONS THEREOF) SUBMITTED FOR PUBLICATION

None

BOOKS (AND SECTIONS THEREOF) PUBLISHED

M.D. Girardeau, "Nonlinear wave equation for decaying states," in Quantum Electrodynamics and Quantum Optics, ed. A.O. Barut (Proceedings of the NATO Advanced Study Institute on Quantum Electrodynamics and Quantum Optics, Boulder, 1983; Plenum Press, New York, 1984), pp. 323-326.

(Note: This work was funded by this ONR contract. There was no other support except for the P.I.'s academic year salary from the University of Oregon.)

PATENTS FILED

None

PATENTS GRANTED

None

INVITED PRESENTATIONS AT TOPICAL OR SCIENTIFIC/TECHNICAL SOCIETY CONFERENCES

None during this period.

HONORS/AWARDS/PRIZES

M.D. Girardeau received a Humboldt Prize (U.S. Senior Scientist Award) from the Alexander von Humboldt-Stiftung. He is using it to fund collaborative research with colleagues at the Max Planck Institut fur Strahlenchemie, Mulheim a.d. Ruhr, West Germany.

HONORS/AWARDS/PRIZES, continued

M.D. Girardeau served on the 1984 Physics Review Panel of the National Research Council (ranking candidates for NRC Postdoctoral Research Associateships at Federal laboratories).

M.D. Girardeau became a Corresponding Member of the Academie Europeenne des Sciences, des Arts, et des Lettres (membership by invitation only).

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